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THE NOMINAL/GENERIC SPECIFIC HEAT PER AVERAGE ATOM CONCEPT FOR CHNO ENERGETIC MATERIALS

James P. Billingsley

System Simulation and Development Directorate
Aviation and Missile Research, Development, and Engineering Center

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This document is a follow on to U.S. Army Micom TR-RD-SS-95-2, AMCOM-TR-RD-SS-98-2, and TR-RD-SS-06-09 that related plane impact shock sensitivity of CHNO energetic materials to specific heat per average atom magnitude and Reactive Temperature (T_R) conditions. Observation of the C_P per average atom versus absolute Temperature (T) plots revealed relatively little difference in magnitude for seven important explosive compounds. Thus, a universal nominal/generic C_P per average atom is proposed for CHNO energetic materials. This report is devoted to substantiating this N/G C_P per average atom concept and illustrating its practical utilization via examples for TNT, HMX, and PBX-9502.

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I. INTRODUCTION

References 1 through 6 contain analyses results for energetic materials impact shock sensitivity correlation with specific heat and reactive temperature magnitudes. Eventually, it turned out that the one-dimensional plane impact shock sensitivity could be correlated rather well with reactive temperature, T_R, magnitudes that governed how much thermal energy an explosive could soak up before a reaction (melting, phase change, detonation) occurred. One basic reason for this is because, for a given temperature, the magnitude of the specific heat per average atom for several important secondary CHNO explosives is almost, or practically, the same value. That is, there is a nominal or generic (N/G) specific heat, C_p, value per average atom as a function of temperature, T, which agrees with the C_p of important CHNO explosives within plus or minus a few percent.

This is remarkable, considering the differences in chemical formula, the number of atoms per molecule (q), and the Molecular Weight (MW) of seven important secondary explosives that are listed in Table 1.

The remainder of this report is devoted to substantiating this N/G C_p per average atom concept and illustrating its practical utilization. This utilization involves the Δ (v.e.)$_{TR}$ concept which is described next in order to clarify certain remarks used in a more detailed discussion of the N/G C_p concept that is presented immediately afterwards in Section III.

II. THE Δ (v.e.)$_{TR}$ CONCEPT

Essentially, the area Δ (v.e.)$_{TR}$ under the C_P versus Temperature (T) plots between temperature limits, Experimental Test Temperature (T_{EXP}) and Reactive Temperature (T_R) is a measure of how much atomic vibratory energy explosives can absorb before a reaction occurs. The reaction may be melting, phase change, decomposition, burning, or even detonation. Thus, to a good approximation, it could be expected that if Δ(v.e)$_{TR}$ amount of energy is suddenly added via impact shock loading, then a reaction may occur.

This Δ (v.e.)$_{TR}$ concept, that impact shock sensitivity or shock induced reactivity of energetic materials could be related to their specific heat (C_P) variation with temperature, was demonstrated in References 1 and 2 for RDX, TETRYL, PETN, TNT, and TATB, which are basic secondary reactive compounds.

In References 3 and 4, the Δ (v.e.)$_{TR}$ ideas were demonstrated for HMX and HNS that are also important basic secondary explosive compounds. The impact shock response of these seven compounds ranges from very insensitive to highly sensitive. Most of these seven basic energetic compounds have been the main ingredient of useful explosive mixtures.

One such mixture is the plastic bonded explosive designated as PBX-9502 that is 95 percent TATB and 5 percent KEL-F800 [7, 8]. PBX-9502 has been rather extensively tested via one-dimensional shock loading at various temperatures, and its thermal characteristics have also been experimentally explored. Consequently, with this much information available, Δ (v.e.)$_{TR}$ concept computations were made for PBX-9502. The exploratory comparative results

for this important energetic material were highly affirmative and are documented in References 5 and 6.

General details of the exploratory computation and experimental data comparisons involved in a general Δ (v.e.)$_{TR}$ assessment are contained in the following paragraphs.

The thermal atomic vibratory energy increment, Δ (v.e.)$_{TR}$, is related to macroscopic critical particle (or mass) velocities (U_{PCR}) and impact shock pressures via Equations (1) through (6).

For certain explosives, a good estimate of the critical particle velocity, U_{PCR} , where a reaction (or detonation) occurs is:

$$U_{PCR1} = \sqrt{\frac{\Delta(\text{v.e.})_{TR}}{m_{AV}}} \tag{1}$$

In some circumstances, a better estimate of the critical particle velocity is:

$$U_{PCR2} = \sqrt{\frac{2\Delta(\text{v.e.})_{TR}}{m_{AV}}} = \sqrt{2} \quad U_{PCR1} \tag{2}$$

Where:

$$\Delta(\text{v.e.})_{TR} = \int_{T_{EXP}}^{T_R} C_p dT \tag{3}$$

	=	Thermal vibratory energy per atom between T_{EXP} and T_R, Gram $(\text{Cm/Sec})^2$.
C_P	=	Specific heat per atom as a function of temperature.
m_{AV}	=	Average mass of an atom in the material, Grams (See References 1, 3, and 5).
T_{EXP}	=	Temperature at which experimental impact shock test are conducted. This is normally room temperature (R T$\approx$ 300°K but can (and should) be done at higher and lower temperatures.
T_R	=	Temperature at which some thermally induced reaction occurs (decomposition, melting, phase change, detonation, etc.).
U_{PCR2}	=	Particle velocity, U_P, such that the shock induced internal energy (e_i) is equal to Δ(v.e,)T_R.
U_{PCR1}	=	Particle velocity, U_P, such that the total shock induced energy (e_t) (kinetic plus internal) is equal to Δ(v.e.)T_R.
e_t	=	$m_{AV}U^2_P$ = total shock energy per average atom.
e_i	=	$\frac{m_{AV}}{2}U_p^2 = e_k =$ internal or kinetic energy of the shocked material per average atom.

Certain explosives, when heated to higher and higher temperatures, melt before they explode, (RDX and TNT, for example). This melting will require that the heat of fusion (ΔH_F) be absorbed by the material at $T=T_{MELT}$ conditions before the temperature will increase [9, 10]. Consequently, if T_{EXP} is less than T_{MELT}, then the total heat absorbed from $T = T_{EXP}$ to $T = T_{EXPL} = T_R$ is:

$$\Delta(\text{v.e.})_{TR} = \int_{T_{EXP}}^{T_{MELT}} C_p dt + \Delta H_F + \int_{T_{MELT}}^{T_{EXPL}} C_p dT. \tag{4}$$

So, for solid energetic materials which melt prior to explosion, then Δ (v.e.)$_{TR}$, as defined by Equation (4) is employed in Equations (1) and (2) to compute U_{PCR1} and U_{PCR2}, respectively. Note that melting is just one example of a phase transformation which may require an enthalpy increment (ΔH_T) to be activated. For example, HMX can exist in different solid polymorphic forms. At a certain temperature, T_T, one form may change to another form if the heat energy of transformation (Δ H_T) is supplied. So, ΔH_T should be added to Equations (3) and (4) if T_R is greater than T_T.

Note that Δ (v.e.)$_{TR}$ as defined by Equations (3) and (4) is actually an enthalpy increment (ΔH). However, it was shown via numerical examples in Appendix B of Reference 1 that, under the experimental C_P acquisition conditions, the pressure times volume terms were minute compared to the C_P integral, $\int_{T_{EXP}}^{T_R} C_p dT$. Thus, $\int_{T_{EXP}}^{T_R} C_p dT$ is essentially all of the internal energy difference caused by thermal stimulation during standard tests at atmospheric pressure to determine the specific heat characteristics.

Once Δ (v.e.)$_{TR}$ and U_{PCR} values are computed, the corresponding shock velocity (U_{SCR}) is ascertained from experimental data for U_S as a function of the particle velocity, U_P. The experimental relationship is usually linear and written empirically as:

$$U_S = C_O + S\, U_P. \tag{5}$$

When $U_P = U_{PCR}$ and $U_S = U_{SCR}$ are determined, the shock pressure is computed from the following well known relation:

$$P_S = \rho_o\, U_S\, U_P, \tag{6}$$

Where ρ_o = Material density (grams/cm^3).

Then U_{PCR} , U_{SCR} , and P_{SCR} may be compared to experimental shock induced reaction threshold information to check the validity of the above Δ (v.e.)$_{TR}$ theory to denote reactive conditions under impact shock stimuli. The numerical computations involved in a Δ (v.e.)$_{TR}$ assessment are straight forward and simple and may be performed with a hand-held calculator.

It must be emphasized that any possible effect of pressure on C_P is not taken into account in the present analysis. The basic idea is that if a quantity of thermal vibration energy, Δ (v.e.)$_{TR}$ under quiescent conditions is able to create a reaction, then the same amount of energy added by an impact shock (e_i or e_t) should also cause some type of reaction. <u>The shock induced reaction</u>

may not be the same type as the temperature induced reaction, but will nevertheless, be a reaction of some kind. It may be less or more severe than the thermally induced reaction.

The C_P unit of calorie/(atom.°K) was employed in plots of C_P versus T information which are shown in this report. This is because the Boltzman constant, k_B=0.33 x 10^{-23} calories/(atom °K) and the maximum C_P at high temperatures for many materials is $3k_B \approx 1.0 \times 10^{-23}$ calories/(atom °K). This is a good mnemonic reference level for comparison purposes. It was noted in Reference 1 that the average C_P per atom for most polymers never reaches the 3 k_B level before a reaction (phase change, melting, glass–to-rubber transition, or even detonation) occurs.

Actually, C_P for some atoms, or combinations of atoms, probably reaches the 3 k_B level and causes a reaction at some T_R. But C_P for a large number of atoms remains much less than 2 k_B. Thus, a large amount of the possible thermal vibratory energy is never activated and the average C_P per atom remains relatively low [11]. In many cases, important temperature induced reactions occur near the average $C_P \approx 2$ k_B level at moderate temperatures (400 to 600°K).

III. THE N/G C_P CONCEPT

It was first documented in Reference 1 that the C_P [Cal/atom °K)] magnitudes (at a given T) for five solid explosive compounds (RDX, TETRYL, PETN, TNT, and TATB) did not differ very much from each other. In Reference 3, it was demonstrated that the C_P for HNS was very close to that for TATB and the Cp for HMX was somewhat less than the TATB C_P at the higher temperatures. Liquid TNT has a larger C_P (at a given T) than these solid energetic compounds. These statements are corroborated by the experimental C_P information exhibited in Figures 1 through 4.

So with two exceptions (melted TNT and δ – HMX), the C_P per atom of five important secondary energetic compounds all had very similar magnitudes near that for TATB. HNS also has the same magnitude and trend (non-linear variation) with temperatures as TATB. The other explosives (RDX, TNT, TETRYL and PETN) C_P have a linear variation (a + b T) over most of their temperature range.

The amount of heat energy these compounds and mixtures can absorb varies considerately. TATB and PBX-9502 can soak up more heat energy, Δ $(v.e.)_{TR}$, than the others by a considerable margin. That is, their reactive temperatures, T_R, were much greater than the other compounds (more than 100°K for TNT, HNS and HMX and over 200°K for TETRYL, PETN, and RDX).

So based on the above remarks and similar remarks in References 1 through 6, a nominal C_P per average atom is proposed and defined as shown in Figure 4 and listed in Table 2. These nominal C_P magnitudes at Room Temperature (RT) and above are very similar to those of TATB, particularly at the high temperatures. Below RT, the proposed N/G C_P magnitudes are very close to (or equal to) the RDX C_P values [13] and TNT C_P values [12] near absolute zero.

IV. COMPARATIVE EXAMPLES

In order to apply the Δ (v.e.)$_{TR}$ concept for threshold U_{PDT} and P_{SDT} prediction, the following experimental information is necessary for the <u>same</u> reactive energetic material.

<u>Thermal Properties</u>:

1. T_R = Some reactive temperature, preferably T_{EXPL}.

2. ΔH = Heat of fusion (ΔH_F, melt) and heat of transformation (ΔH_T). If $T_R \geq T_{MELT}$ or T_{TRAN}.

3. C_P = Specific heat as function of temperature, T.

<u>Impact Shock Related Properties</u>:

1. ρ_o = Material density (gram/cm^3) at each test condition (T_{EXP}).

2. U_S = Shock velocity as a function of U_P for each test condition at T_{EXP}.

Of all this desirable information, $C_P = f(T)$ is possibly the most difficult to obtain. This section will demonstrate that the N/G C_P will suffice if experimental C_P data is not available.

So in this section, computation of Δ (v.e.)$_{TR}$, U_{PCR} , and P_{SCR} are made for three explosives by using the proposed N/G C_P listed in Table 2 and shown in Figure 4. This information is compared to similar results, documented in References 1, 3, and 5, that were computed from the experimental C_P data for each of the three explosives.

The three explosives selected for comparison are TNT, PBX-9502, and HMX that encompasses both the high and low experimental C_P magnitudes (compared to the proposed N/G C_P). The following relations are employed as comparative measures:

$$\frac{\Delta U_{PCR}}{U_{PCR}(EXP)} = \frac{U_{PCR}(N/G) - U_{PCR}(EXP)}{U_{PCR}(EXP)} \text{ X } 100.0 \qquad (7)$$

$$= \text{percent difference in } U_{PCR}$$

$$\frac{\Delta P_{SCR}}{P_{SCR}(EXP)} = \frac{P_{SCR}(N/G) - P_{SCR}(EXP)}{P_{SCR}(EXP)} \text{ X } 100.0 \qquad (8)$$

$$= \text{percent difference in } P_{SCR}$$

Where:

U_{PCR} (EXP)	=	U_{PCR} from experimental C_P
U_{PCR} (N/G)	=	U_{PCR} from N/G C_P
P_{SCR} (EXP)	=	P_{SCR} from experimental C_P
P_{SCR} (N/G)	=	P_{SCR} from N/G C_P

A. TNT

The TNT experimental C_P per average atom is somewhat larger than the proposed N/G C_P. This is particularly true for liquid TNT. In fact, liquid TNT has a larger C_P per average atom than any of the other CHNO explosive C_P magnitudes that are plotted in Figures 1 through 4.

Because of TNT's large liquid C_P situation, two different cases where investigated. These are defined as follows:

<u>Case 1.</u>	–	Liquid C_P included in Δ (v.e.)$_{TR}$ computations
T_{EXP}	=	25°C = 298°K = RT
T_R	=	300°C = 573°K = T_{EXPL}
<u>Case 2.</u>	–	Liquid C_P not included in Δ (v.e.)$_{TR}$ computations
T_{EXP}	=	18°C = 291°K = RT
T_R	=	80.5°C = 353.5° = T_{MELT}

For both cases, ΔH_F (melt) was included in the Δ (v.e.)$_{TR}$ computations.

Tables 3 and 4 contain excerpted results from Reference 1 for TNT with the experimental C_P data input for both Case 1 and Case 2 conditions. For Case 2, some supplementary computations were required in Table 4 that were appropriate for pressed TNT.

Tables 5 and 6 contain similar results for both Case 1 and Case 2 that were computed with the proposed N/G CP.

Table 7 lists the U_{PCR} and P_{SCR} results from both cases and the percentage differences calculated via Equations (7) and (8). The percentage computations show that for:

<u>Case 1.</u>

(a) The U_{PCR} results from the proposed N/G C_P values are 7 percent lower that the U_{PCR} results computed from the experimental C_P magnitudes.

(b) The P_{SCR} results from the proposed N/G C_P values are as much as 10 percent lower than P_{SCR} results computed from the experimental C_P magnitudes.

Case 2.

(a) The U_{PCR} results from the proposed N/G C_P values are 2.0 percent lower than the U_{PCR} results computed from the experimental C_P magnitudes.

(b) The P_{SCR} results from the proposed N/G C_P values are nearly 3.0 percent lower than the P_{SCR} results computed from the experimental C_P magnitudes.

Figures 5 and 6 illustrate the comparative magnitudes for U_{PCR} and P_{SCR}, respectively.

B. PBX-9502

The PBX-9502 experimental C_P per average atom and the proposed N/G C_P per average atom have similar magnitudes as shown in Figures 2, 3, and 4.

Tables 8 and 9 list excerpted information from Reference 5 for PBX-9502 with the experimental C_P data input for the following test temperature conditions:

T_{EXP} = -55°C/218°K, 20°C/293°K, 75°C/348°K, and 252°C/525°K

T_R = 396°C/669°K = T_{EXPL} for all T_{EXP} conditions

This was done without ΔH_T (melt) included in the Δ (v.e.)$_{TR}$ computations.

Tables 10 and 11 contain similar results for these four conditions computed with the proposed N/G C_P. Table 12 lists the U_{PCR} and P_{SCR} results from both sets of computation and the percentage differences calculated via Equations (7) and (8).

The percentage comparisons indicate that:

(a) The U_{PCR} values from the proposed N/G C_P data are from 0.06 to 1.54 percent lower than U_{PCR} values computed from the experimental C_P magnitudes.

(b) The P_{SCR} values from the proposed N/G C_P data are from 0.09 to 2.09 percent lower that P_{SCR} values computed from the experimental C_P magnitudes.

Figures 7 and 8 illustrate this information for PBX-9502 in a comparative manner. Only U_{PCR1} and P_{SCR1} computed magnitudes are shown in Figures 7 and 8, respectively. However, the percentage differences for U_{PCR2} are the same as those for U_{PCR1}. The percentage differences for P_{SCR2} are practically the same as for P_{SCR1}.

C. HMX

The experimental C_P per average atom for HMX is less than the proposed N/G C_P for a given temperature, T. Even though the HMX C_P is somewhat less than the C_P for the other six explosive compounds, shown in Figures 1 through 4, HMX is not extremely heat sensitive because its reactive temperatures are relatively high. In fact, HMX is an abbreviation for Higher Melting Explosive. Its explosion (T_{EXPL}) or deflagration (T_{DELF}) temperatures are close to its melting (T_{MELT}) temperature.

Tables 13 and 14 contain excerpted information from Reference 3 for HMX with the experimental C_P data input for the following test temperature conditions:

T_{EXP} = 27°C = 300°K = RT

T_R = 287°C = 560°K = T_{DEF} (Deflagration)

This was done with ΔH_T ($\beta \rightarrow \delta$) included in the Δ (v.e.)$_{TR}$ computations.

Tables 15 and 16 contain similar results for this condition computed with the proposed N/G C_P. Table 17 lists the U_{PCR} and P_{SCR} results from both sets of computations and the percentage differences calculated via Equations (7) and (8).

The percentage comparisons show that:

(a) The U_{PCR} values from the proposed N/G C_P data are 2.43 percent higher than U_{PCR} values computed from the experimental C_P magnitudes.

(b) The P_{SCR} values from the proposed N/G C_P data are from 3.07 to 3.28 percent higher than the P_{SCR} values computed from the proposed N/G C_P values.

Figures 9 and 10 illustrate this information for HMX in a comparative manner.

V. DISCUSSION

The examples (TNT and HMX) were selected because their experimental C_P was high (TNT) or low (HMX) compared to five other CHNO energetic compounds and one energetic mixture (PBX-9502). TNT is considered an extreme example because of its rather large C_P and sizeable ΔH_F for the melted (liquid) condition, so two cases were considered for TNT.

Case 1 had a rather large T_R (300°C/573°K) where the experimental/extrapolated C_P had to be included in the Δ (v.e.)$_{TR}$ computations. This case corresponds to an assessment for cast TNT [1]. For Case 1, the difference in U_{PCR} ($\Delta U_{PCR} / \Delta U_{PCR}(EXP)$), was -7.0 percent and the maximum difference in P_{SCR} ($\Delta P_{SCR} / \Delta P_{SCR}(EXP)$) was about a-10.0 percent.

Case 2 for TNT had a smaller T_R (80.5°C/353.5°K) corresponding to T_{MELT}. So computations for Δ (v.e.)T_R did not include the C_P for liquid TNT. This case corresponds to an assessment for pressed TNT [1]. For Case 2, the difference in the U_{PCR} computations was about a -2.0 percent and the maximum difference in P_{SCR} was about a -3.0 percent.

As expected, there was little difference in Δ (v.e.)T_R U_{PCR} and P_{SCR} computed via the PBX-9502 C_P and the proposed N/G C_P. From Table 12, this difference was no greater than about -1.5 percent in U_{PCR} and about -2.0 percent in P_{SCR}.

Likewise, from Table 17 for HMX, the difference in U_{PCR} was about +2.4 percent and the maximum difference in P_{SCR} was about +3.3 percent.

Consequently, excluding Case 1 for TNT where the large liquid C_P had to be included in the U_{PCR} (EXP) and P_{SCR} (EXP) computations, then for TNT (Case 2), PBX-9502, and HMX, the maximum percentage differences between the (EXP) C_P and (N/G) C_P results are bounded by:

$$\frac{\Delta U_{PCR}}{U_{PCR}(EXP)} = \frac{U_{PCR}(N/G) - U_{PCR}(EXP)}{U_{PCR}(EXP)} \text{ X } 100.0 < |\, 2.5\% \,| \qquad (9)$$

$$\frac{\Delta P_{SCR}}{P_{SCR}(EXP)} = \frac{P_{SCR}(N/G) - P_{SCR}(EXP)}{P_{SCR}(EXP)} \text{ X } 100.0 < |\, 3.5\% \,| \qquad (10)$$

These small differences provide considerable credibility for the proposed N/G C_P per average atom concept for most CHNO energetic materials.

What is the value (or usefulness) of the nominal C_P concept for CHNO energetic materials? Answers are:

1. In References 1 through 4 and the present report, it has already been employed, as part of the Δ (v.e.)$_{TR}$ concept, to quantitatively explain or show that:

   (a) As $T_R = T_{EXPL}$ increases, so does insensitivity to impact shock loads [1 through 4].

   (b) As T_{EXP} increases above RT for a given T_R, less impact shock loading (P_S or U_P) is required (compared to RT conditions) to cause explosive reactions. [1 and present report].

   (c) As T_{EXP} decreases below RT for a given T_R, more impact shock loading (P_S or U_P) is required (compared to RT conditions) to cause an explosive reaction. [1 and present report].

2. Some idea of the impact shock sensitivity of new CHNO explosives under development could be acquired from minimum thermal data ($T_R = T_{EXPL}$ estimates) and minimum Hugoniot impact shock data (U_S, U_P). This could proceed similar to the example for PBX-9502 with the nominal C_P. However, certain Hugoniot (U_S, U_P) data may not be readily available and would require estimation.

3. The N/G C_P could be employed in numerical computations of impact shock induced temperatures for CHNO explosives under development where $C_P = f$ (T) may not be known or well defined.

4. The N/G C_P could be employed in analytical/numerical computations of heat transfer in CHNO energetic materials where $C_P = f$ (T) may be unknown.

VI. RECOMMENDATIONS

Most of the recommendations stated in Reference 1 for C_P and detonation threshold information acquisition are still valid. In particular, experimental C_P data acquisitions for the following conditions are still needed.

1. C_P at low cryogenic temperatures up to RT for HMX and TATB.

2. C_P for different densities (ρ_o) up to, and including, crystals at TMD for TNT, RDX, HMX, and TATB.

The presently proposed N/G CP magnitude, in certain temperature regions, may require some revisions if the above information was judiciously incorporated into the existing data gaps.

In References 17 and 18 it is shown that specific heat for many inert polymers can be calculated as an additive molar property from certain molecular groups. It is recommended that this type of analysis be applied to the computation of C_P for at least one or two of the seven basic energetic polymer compounds listed in Table 1. TNT and RDX are suggested because experimental C_P data are available for a comparative check from cryogenic to melting temperatures. If successful, the analysis could provide information and insight about the specific heat contribution of the different atomic or sub-molecular groups within the basic large molecule which contains more than 20 atoms.

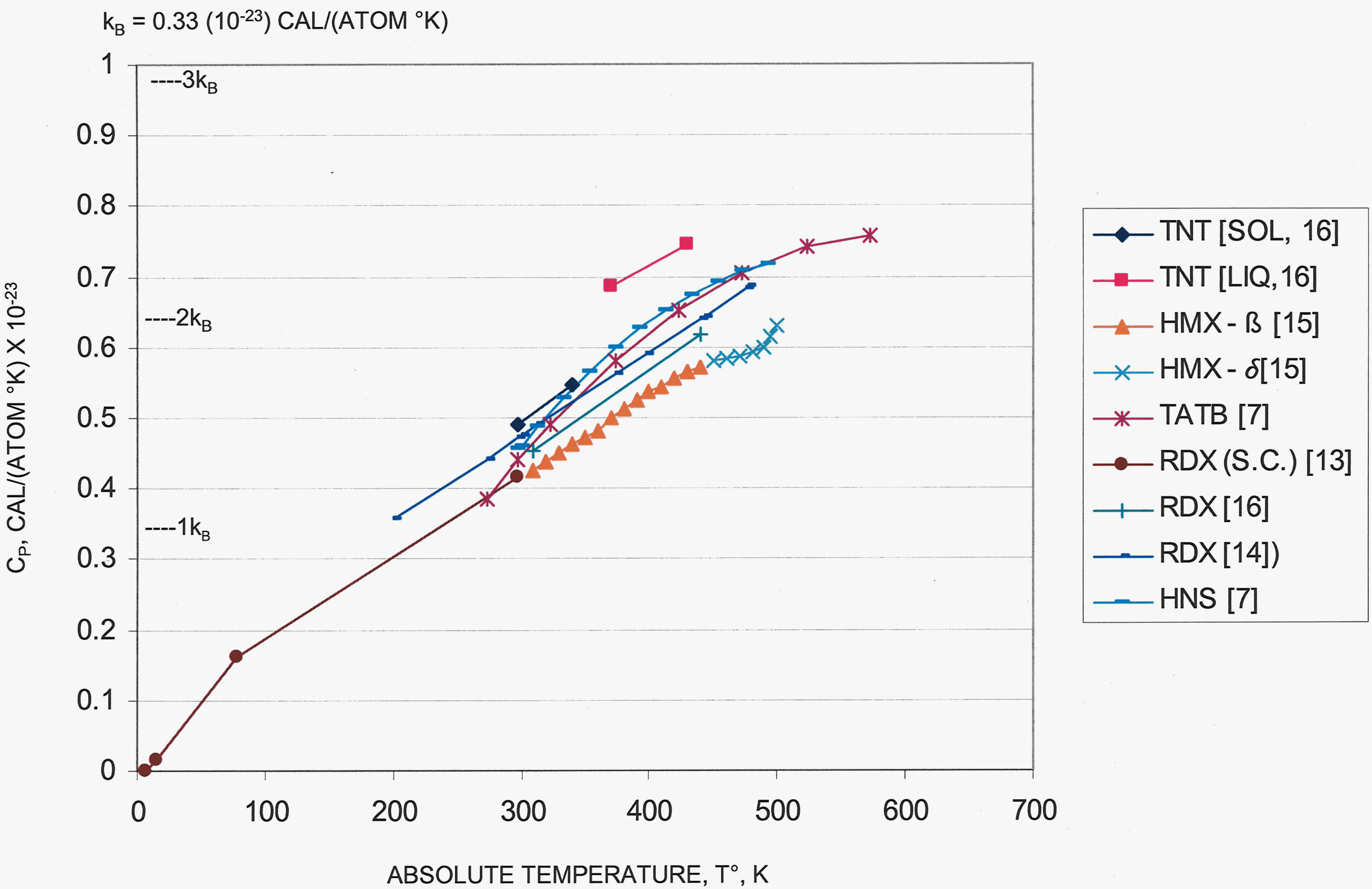

Figure 1. The Specific Heat Per Average Atom for TATB, RDX, TNT, HMX, and HNS

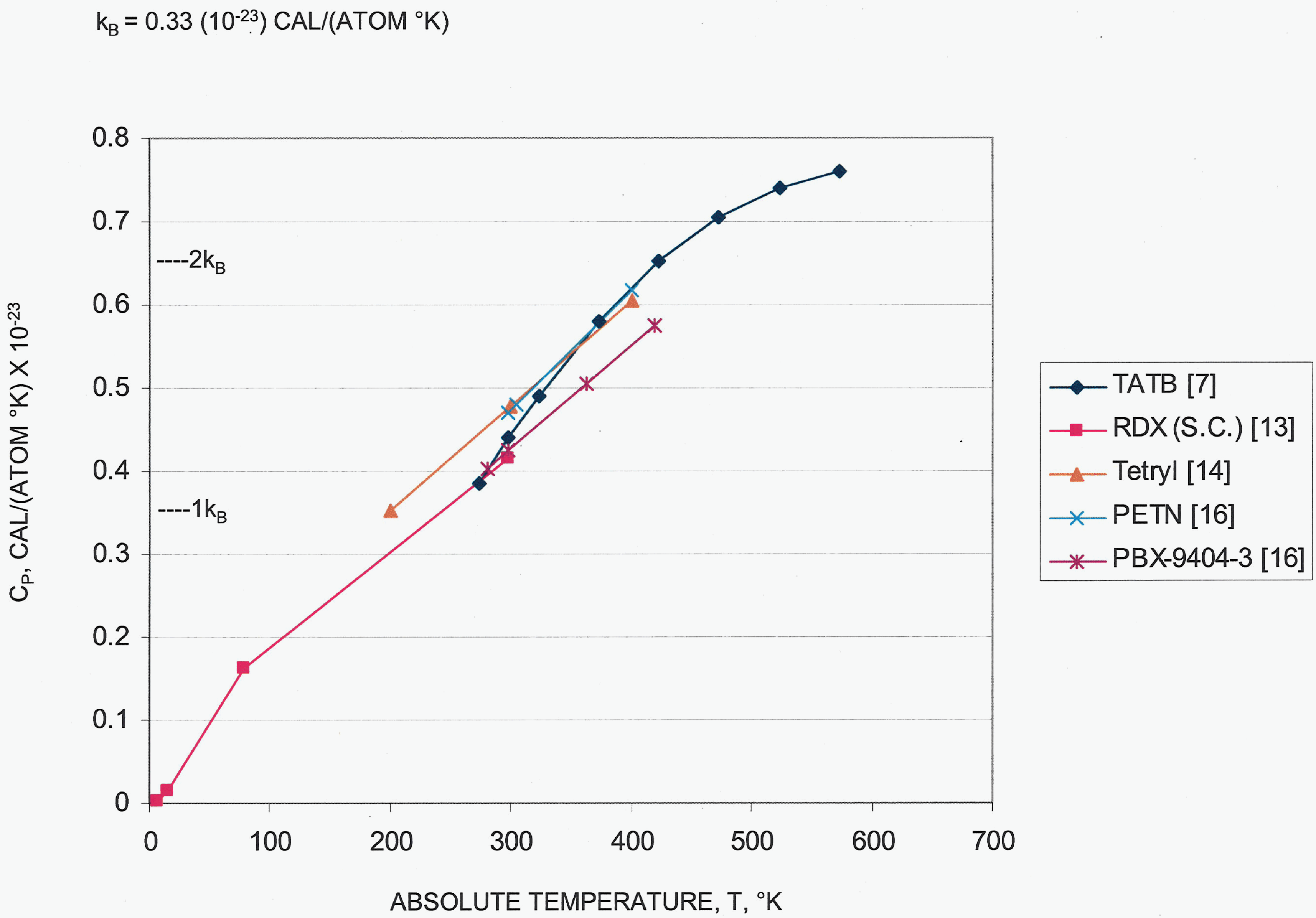

Figure 2. The Specific Heat Per Average Atom for TATB, RDX, TETRYL, PETN, and PBX-9404-3

$k_B = 0.33\ (10^{-23})$ CAL/(ATOM °K)

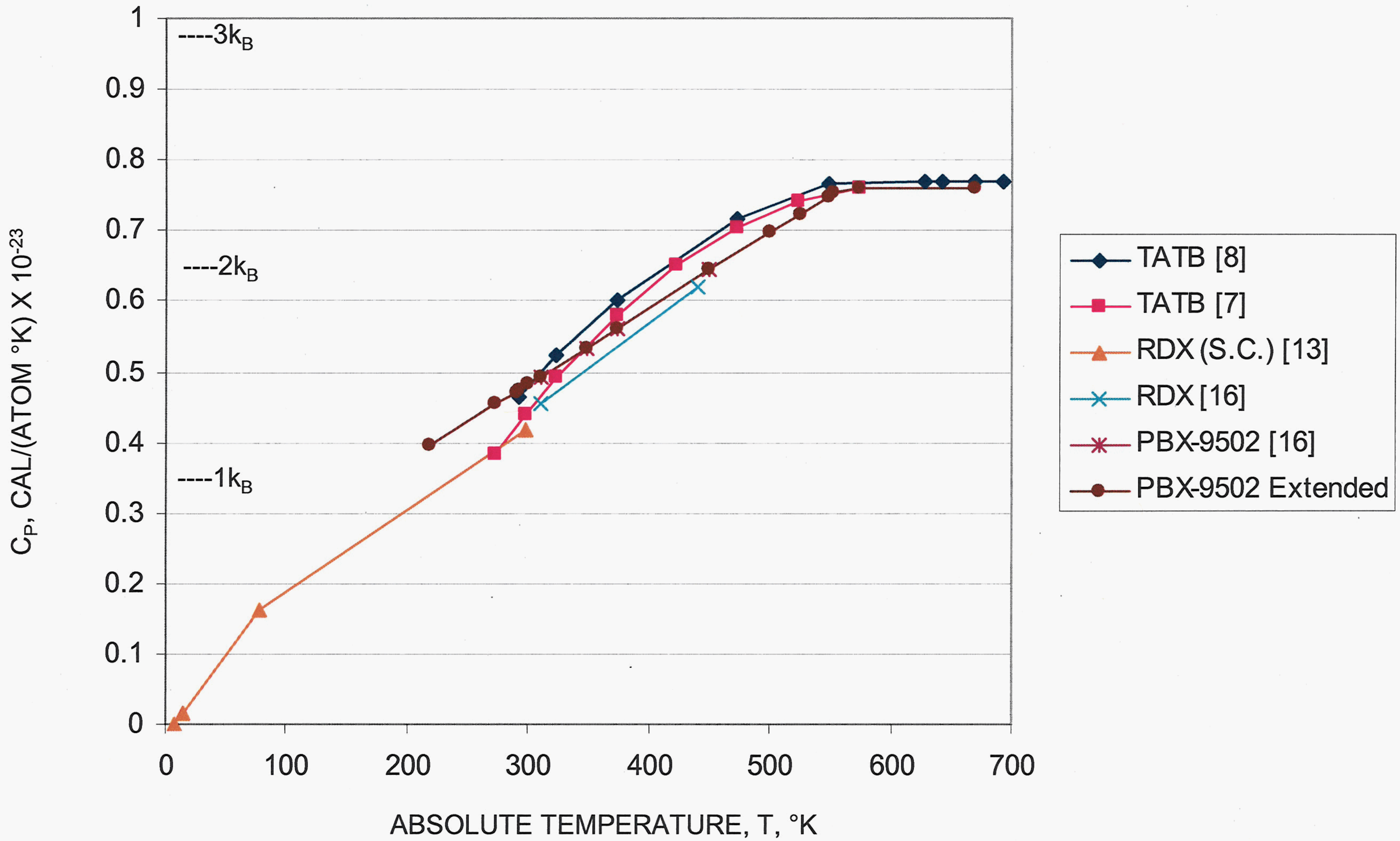

Figure 3. The Specific Heat Per Average Atom for TATB, PBX-9502, and RDX

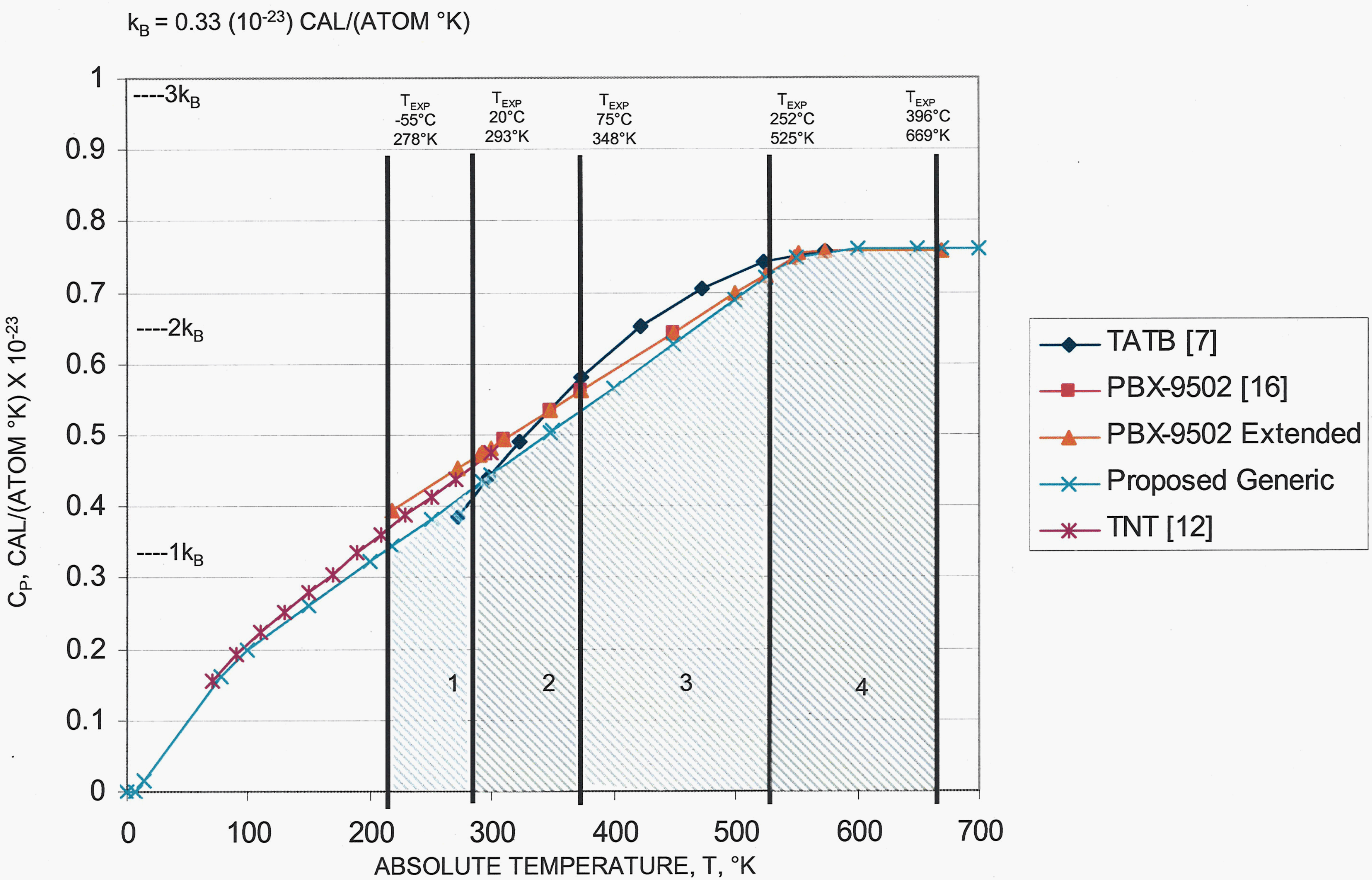

Figure 4. The Specific Heat Per Average Atom for TATB, PBX-9502, TNT, and the Proposed Generic Cp

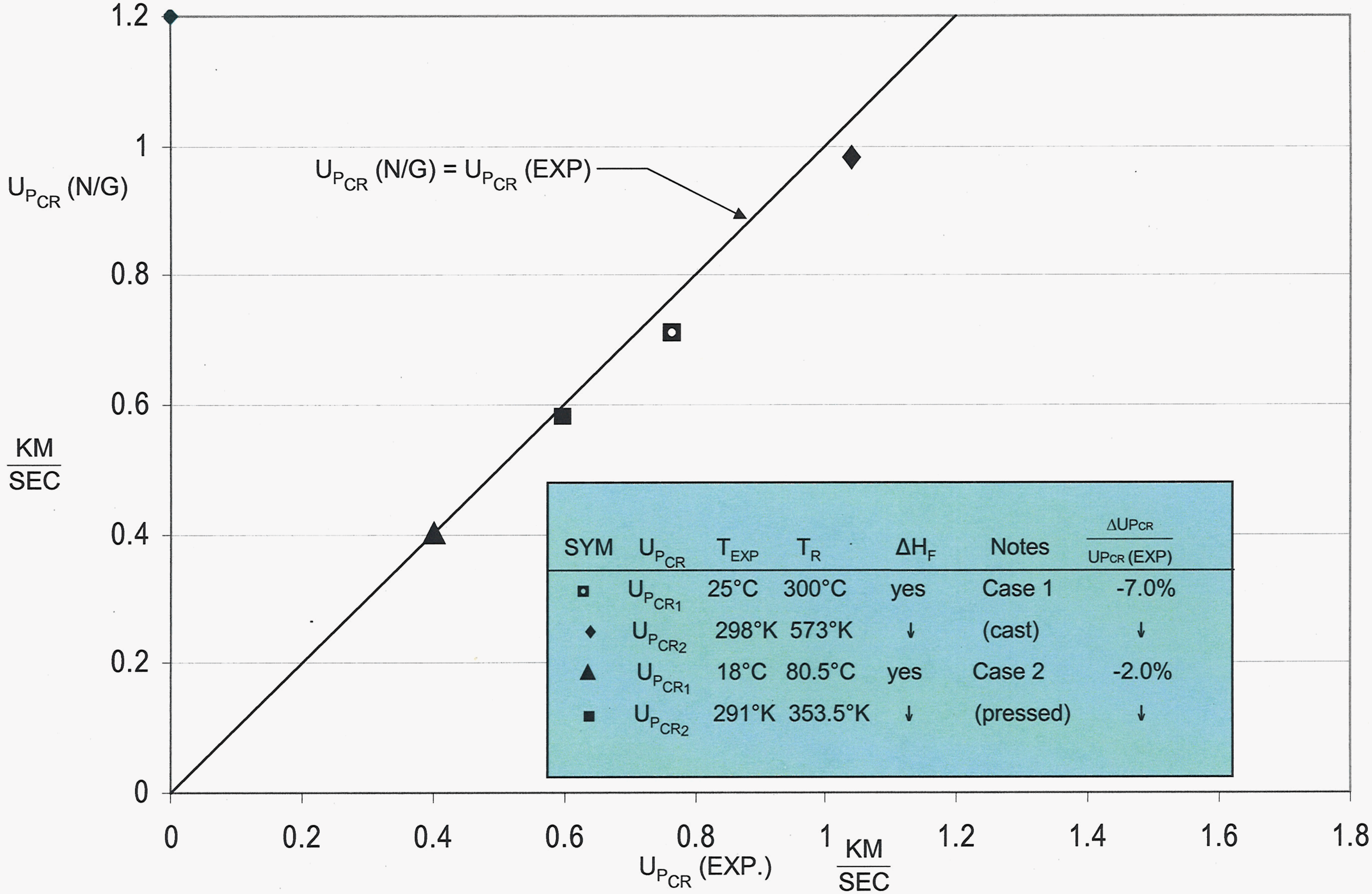

Figure 5. $U_{P_{CR}}$ (N/G) and $U_{P_{CR}}$ (EXP) Comparison for TNT

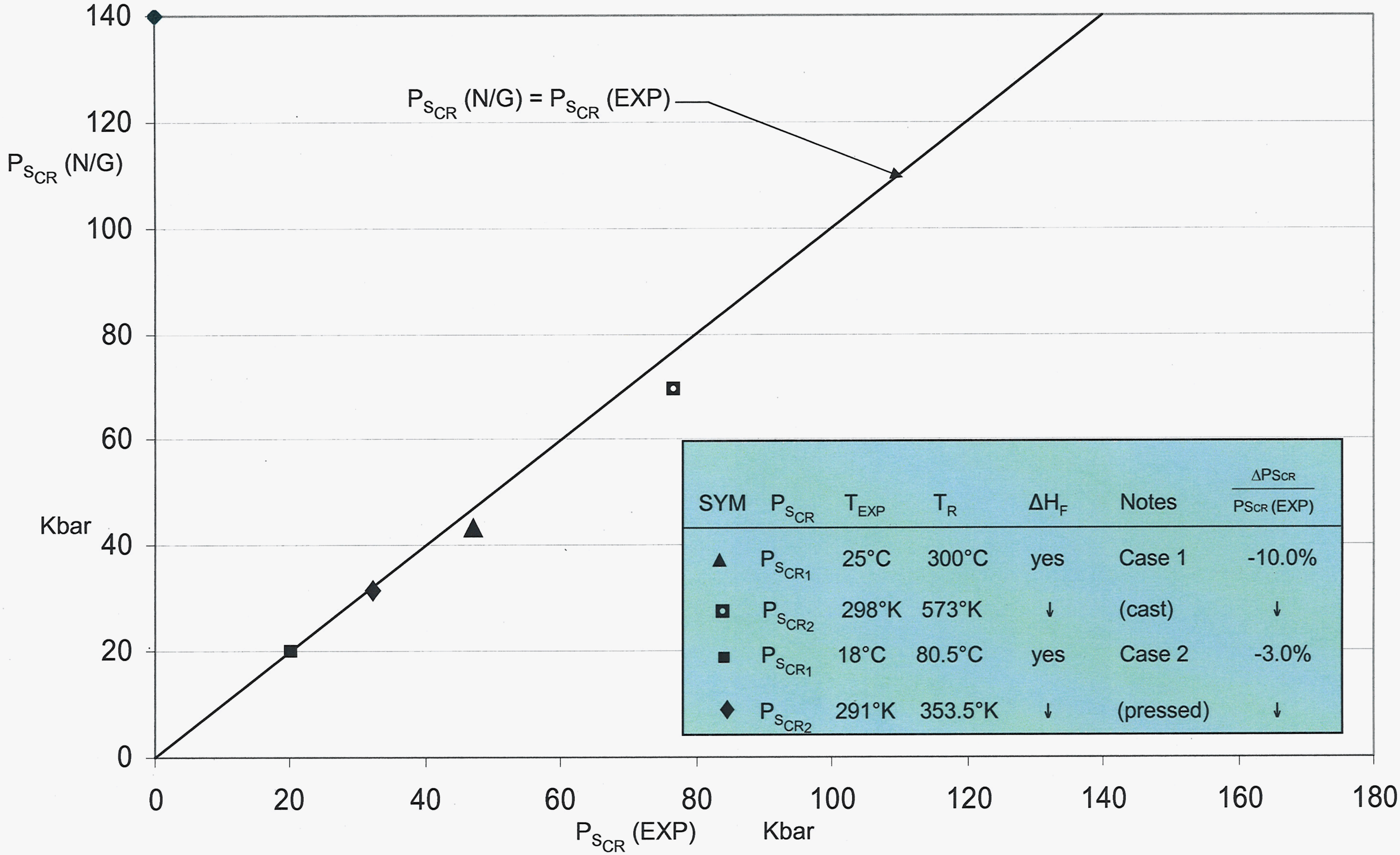

Figure 6. $P_{S_{CR}}$ (N/G) and $P_{S_{CR}}$ (EXP) Comparison for TNT

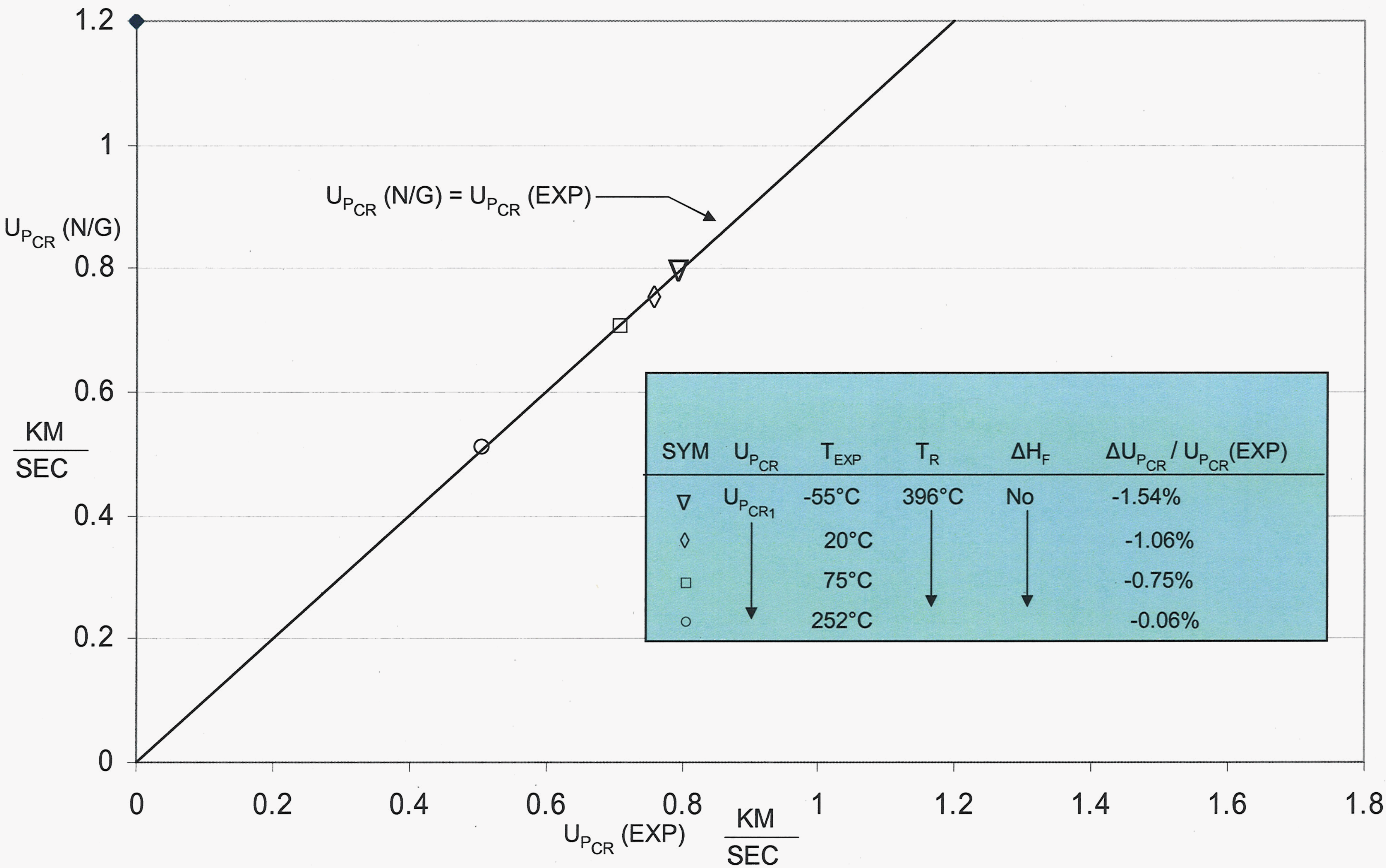

Figure 7. $U_{P_{CR}}$ (N/G) and $U_{P_{CR}}$ (EXP) Comparison for PBX-9502

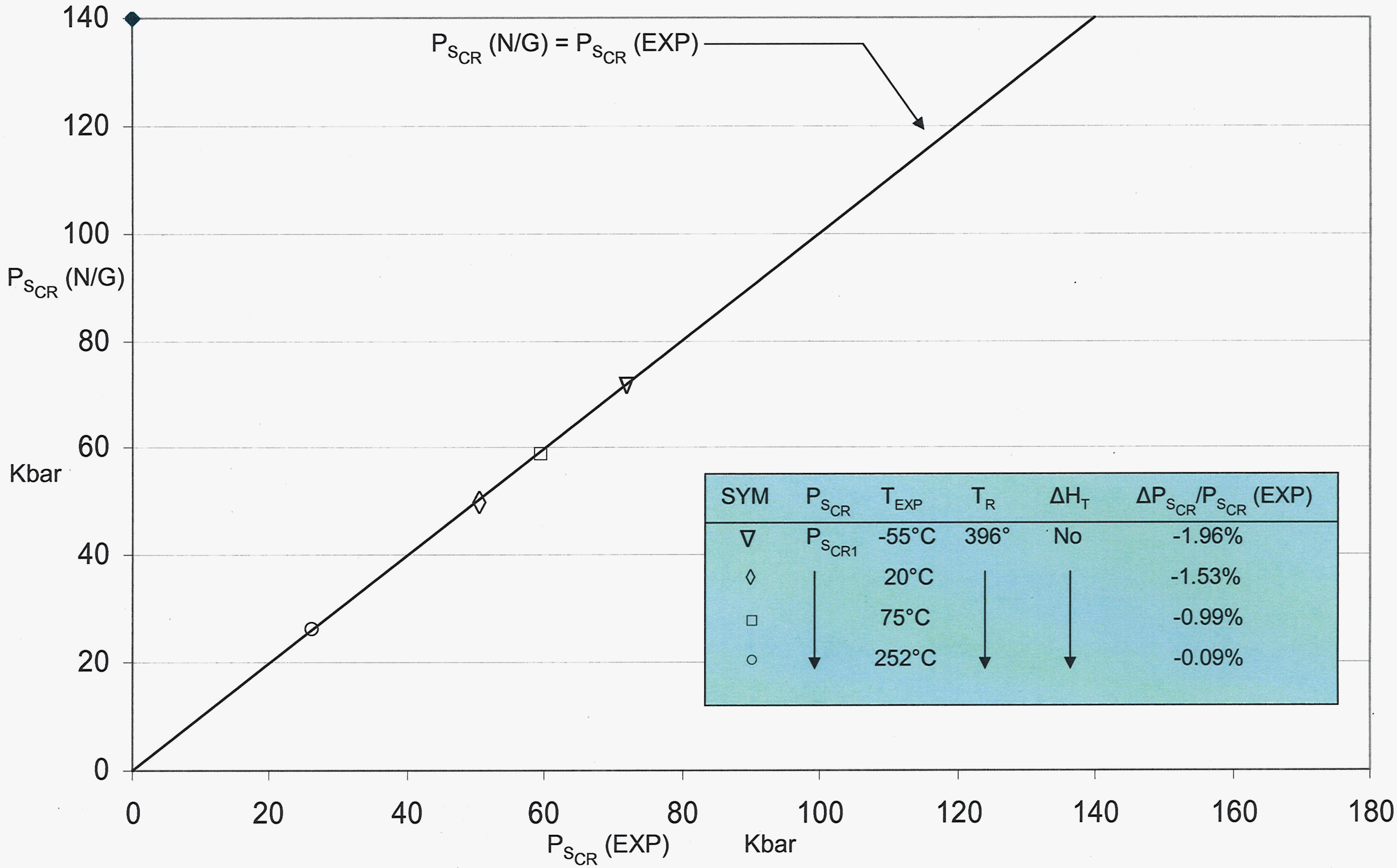

Figure 8. $P_{S_{CR}}$ *(N/G) and* $P_{S_{CR}}$ *(EXP) Comparison for PBX-9502*

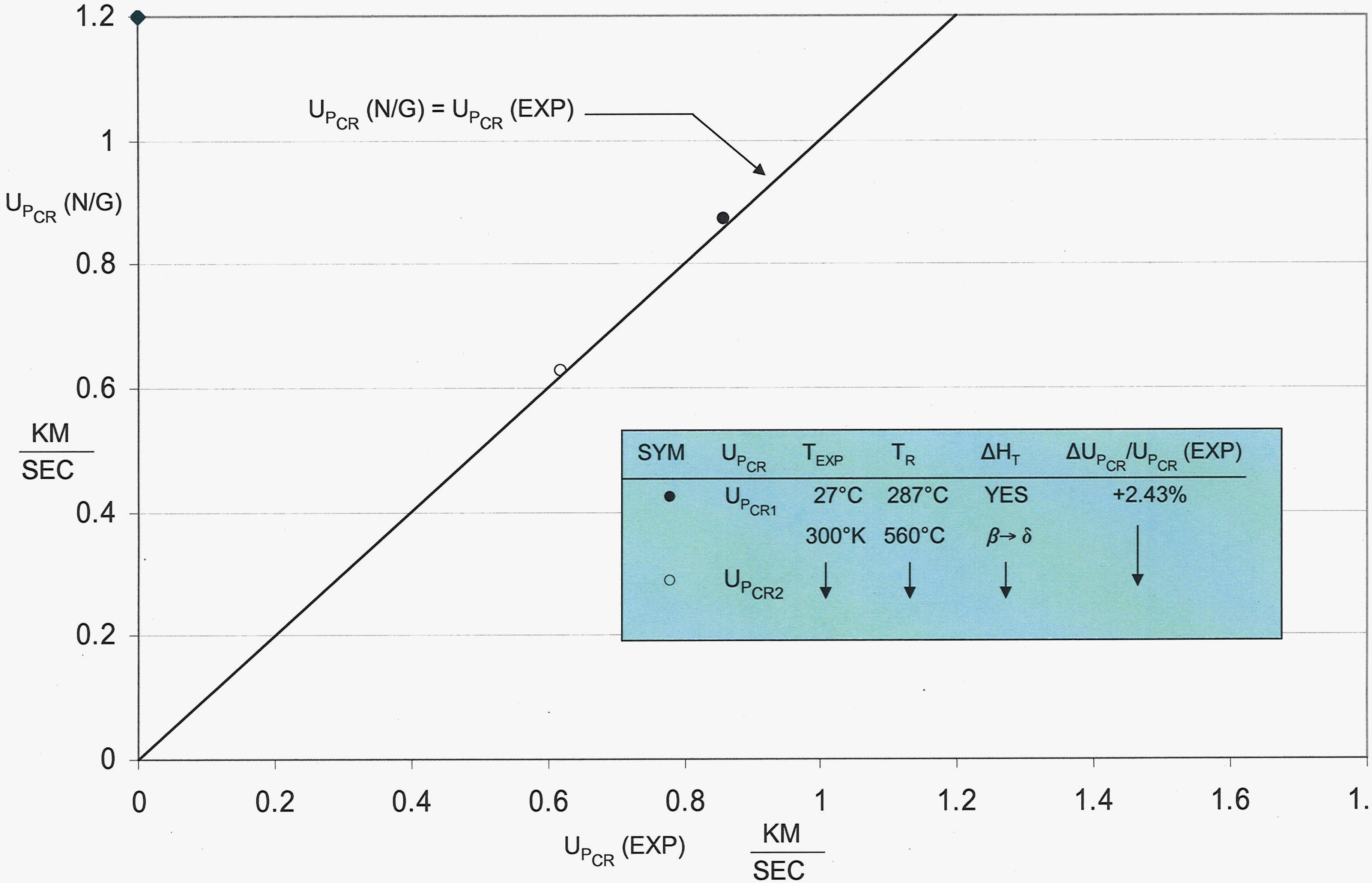

Figure 9. $U_{P_{CR}}$ (N/G) and $U_{P_{CR}}$ (EXP) Comparison for HMX

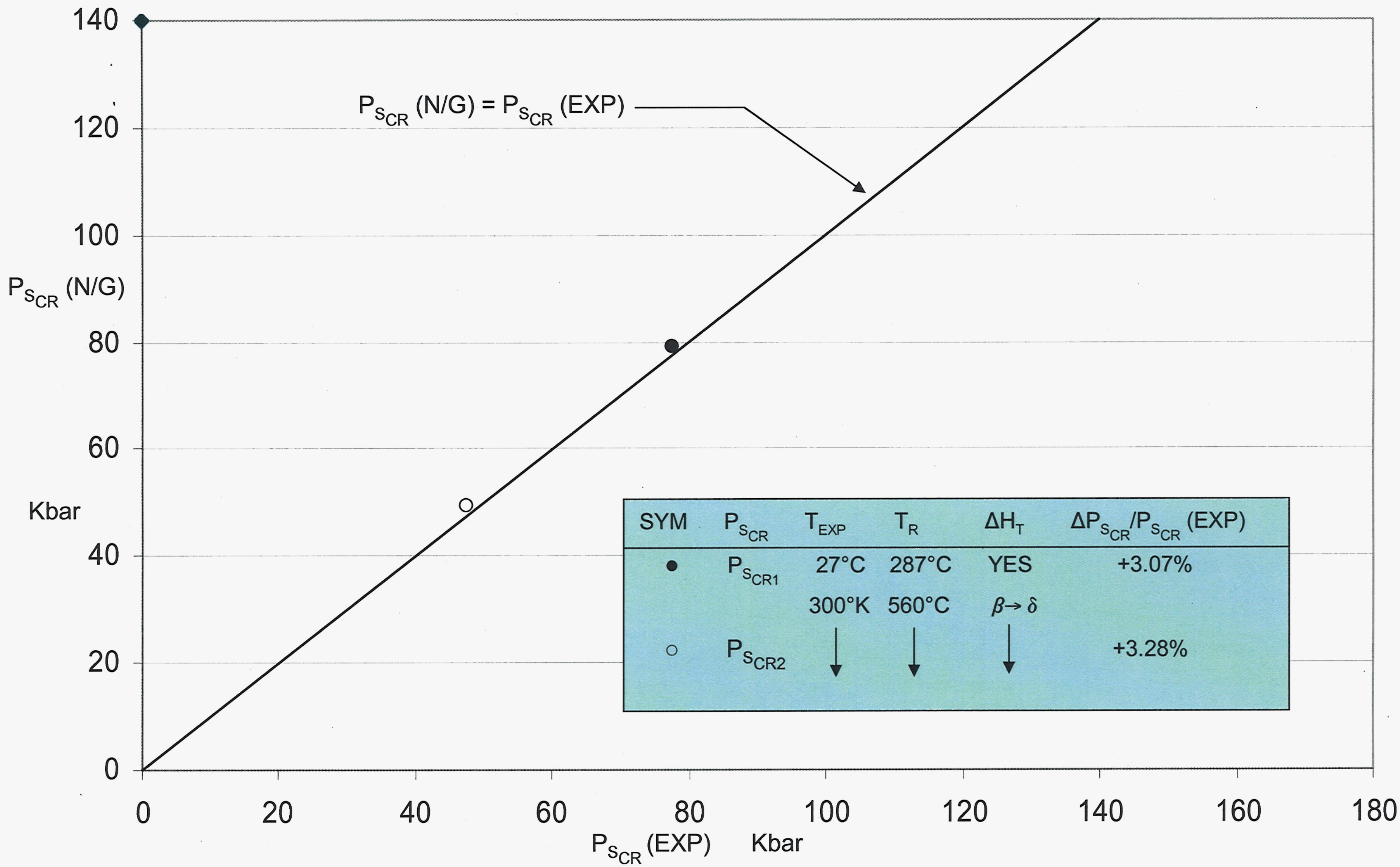

Figure 10. $P_{S_{CR}}$ (N/G) and $P_{S_{CR}}$ (EXP) Comparison for HMX

Table 1. Information for Seven Important Secondary Explosive Compounds

ITEM	CHEMICAL FORMULA $= C_i H_j N_k O_\ell$	NAPM $= i + j + k + \ell$	MW	M_{AV}	NAMW $= \frac{MW}{m_{av}}$	TMD $= \rho_{\circ\ MAX}$	T_{MELT} (MELT)	T_{EXPL} (EXPLODE)	ΔH_T per average atom	REF.*
~	~ ~ ~	q	G/Mole	G/Atom	$N_{AV}\ q$	G/CC	°C/°K	°C/°K	G(cm/sec²)	~
TETRYL	$C_7 H_5 N_5 O_8$	25	287.0	1.9072×10^{-23}	$150.837 \times 10^{+23}$	1.73	129.5/402.5	185.0/458.0	0.15240×10^{-13} (melt)	[1]
PETN	$C_5 H_5 N_4 O_{12}$	29	316.2	1.8102×10^{-23}	$174.677 \times 10^{+23}$	1.78	141.3/414.3	202.0/475.0	0.27569×10^{-13} (melt)	[1]
TNT	$C_7 H_5 N_3 O_6$	21	227.1	1.7959×10^{-23}	$126.451 \times 10^{+23}$	1.654	80.5/353.8	300.0/573.0	0.17358×10^{-13} (melt)	[1]
RDX	$C_3 H_6 N_6 O_6$	21	222.1	1.7563×10^{-23}	$126.459 \times 10^{+23}$	1.806	204.0/477.0	$\approx T_{MELT}$?	0.28217×10^{-13} (melt)	[1]
HMX	$C_4 H_8 N_8 O_8$	28	296.2	1.7563×10^{-23}	$168.6228 \times 10^{+23}$	1.905	282.0/555.0	287/560 T_{DEFL}	0.05515×10^{-13} $\beta \rightarrow \delta$	[3]
HNS	$C_{14} H_6 N_6 O_{12}$	38	450.1	1.9674×10^{-23}	$228.7791 \times 10^{+23}$	1.740	318.0/591.0	321.0/594.0	~	[3]
TATB	$C_6 H_6 N_6 O_6$	24	258.2	1.7861×10^{-23}	$144.5608 \times 10^{+23}$	1.938	300.0/573.0 Sublime	409.0/682.0	~	[1]

*See Sources cited in References 1 and 3.

Table 2. The Generic C_P Per Average Atom for CHNO Explosives

T	T	C_P	Remarks
°K	°C	$\frac{\text{Cal}}{\text{Atom - °K}}$	~
0.0	-273	0.0000	↑
7.0	-266	$0.001344(10^{-23})$	Same as
15.0	-258	$0.01463(10^{-23})$	RDX (S.C.) Ref. [13]***
78.0	-195	$0.1629(10^{-23})$	↓
100.0	-173	$0.2000(10^{-23})$	
150.0	-123	$0.2611(10^{-23})$	
200.0	-73	$0.3222(10^{-23})$	
218.0	-55	$0.3442(10^{-23})$	
250.0	-23	$0.3833(10^{-23})$	See Note 1
293.0	20	$0.4359(10^{-23})$	
300.0	27	$0.4444(10^{-23})$	
348.0	75	$0.5031(10^{-23})$	
350.0	77	$0.5056(10^{-23})$	
400.0	127	$0.5667(10^{-23})$	
450.0	177	$0.6277(10^{-23})$	
500.0	227	$0.6889(10^{-23})$	
525.0	252	$0.7194(10^{-23})$	
550.0	277	$0.7500(10^{-23})$	
600.0	327	$0.7600(10^{-23})$	↑
650.0	377	$0.7600(10^{-23})$	Same as
669.0	396	$0.7600(10^{-23})$	TATB
700.0	427	$0.7600(10^{-23})$	↓

***S.C. = Single Crystal

Note 1: C_P [Cal/(Atom - °K) $= [0.2000 + 0.001222\ (T - 100)]\ 10^{-23}$

$$= [0.07780 + 0.001222\ T\ (°K)]\ 10^{-23}$$

For: $100 \leq T\ (°K) \leq 550$

Table 3. Computation of Up_{CR1} and Up_{CR2} From Experimental C_P for TNT

ITEM ~	m_{AV}	T_{EXP}	T_R	Remarks	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	ΔH_T	$\Delta(v.e.)_{TR}$	$\frac{\Delta(v.e)_{TR}}{m_{av}}$	Up_{CR1}	Up_{CR2}
~	Grams *10-23	°C °K	°C °K	~	Cals *10-23	Joules *10-23	$G\left(\frac{Cm}{Sec}\right)^2$ *10-13	$G\left(\frac{Cm}{Sec}\right)^2$ *10-13	$G\left(\frac{Cm}{Sec}\right)^2$ *10-13	$\left(\frac{Cm}{Sec}\right)^2$ *10+10	$\frac{Km}{Sec}$	$\frac{Km}{Sec}$
TNT	1.796	25 298 RT	300 573 T_{EXPL}	With Δ HT (melt)	200.071	837.097	0.837097	0.17358 (melt)	1.01068	0.56277	0.7502	1.0609
TNT	1.796	18 291 RT	80.5 353.5 T_{MELT}	With Δ H_T (melt)	32.526	136.089	0.136089	0.17358 (melt)	0.0967	0.17242	0.4152	0.5872

Note: This information is from Reference 1.

Table 4. Computation of Us_{CR} and Ps_{CR} From Experimental C_P for TNT

ITEM ~	T_{EXP} °C ° K	ρ_O $\frac{\text{Grams}}{\text{Cm}^3}$	C_O $\frac{\text{Km}}{\text{Sec}}$	S ~	Remarks	U_{CR1} $\frac{\text{Km}}{\text{Sec}}$	Us_{CR1} $\frac{\text{Km}}{\text{Sec}}$	Ps_{CR1} Kbars	T_R °C °K	U_{CR2} $\frac{\text{Km}}{\text{Sec}}$	Us_{CR2} $\frac{\text{Km}}{\text{Sec}}$	Ps_{CR2} Kbars
TNT* (S.C.)	25 298 (RT)	1.654 (TMD)	2.30	2.25	With ΔH_T (melt)	0.7502	3.9880	49.48	300 573 T_{EXPL}	~	~	~
TNT* (S.C.)	25 298 (RT)	1.654 (TMD	3.00	1.58	With ΔH_T (melt)	~	~	~	300 573 T_{EXPL}	1.0609	4.6762	82.06
TNT* (CAST) ↓	25 298 (RT)	1.614	2.39	2.05	With ΔH_T (melt)	0.7502	3.9279	47.56	300 573 T_{EXPL}	1.0609	4.5648	78.16
TNT** (PRESSED) ↓	18 291 (RT)	1.635	2.08	2.35	With ΔH_T (melt)	0.4152	3.0557	20.74	80.5 353.5 T_{MELT}	0.5872	3.4599	33.22

* Reference 1

** Present computation

Table 5. Computation of Up_{CR1} and Up_{CR2} From N/G C_P for TNT

ITEM ~	m_{AV}	T_{EXP}	T_R	Remarks	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	ΔH_T	$\Delta(v.e.)_{TR}$	$\frac{\Delta(v.e)_{TR}}{m_{av}}$	U_{CR1}	U_{CR2}
~	Grams $*10^{-23}$	°C °K	°C °K	~	Cals $*10^{-23}$	Joules $*10^{-23}$	$G\left(\frac{Cm}{Sec}\right)^2 *10^{-13}$	$G\left(\frac{Cm}{Sec}\right)^2 *10^{-13}$	$G\left(\frac{Cm}{Sec}\right)^2 *10^{-13}$	$\left(\frac{Cm}{Sec}\right)^2 *10^{+10}$	$\frac{Km}{Sec}$	$\frac{Km}{Sec}$
TNT	1.796	25 298 (RT)	300 573 T_{EXPL}	with ΔH_T (melt)	167.4768	700.7229	0.7007229	0.17358 (melt)	0.87430	0.48681	0.6977	0.9867
TNT	1.796	18 291 (RT)	80.5 353.5 T_{MELT}	with ΔH_T (melt)	29.4743	123.3205	0.1233205	0.17358 (melt)	0.29690	0.16531	0.4066	0.5750

Table 6. Computation of $U_{S_{CR}}$ and $P_{S_{CR}}$ From N/G C_P for TNT

ITEM ~	T_{EXP} °C ° K	ρ_O Grams/Cm^3	C_O Km/Sec	S ~	Remarks	U_{CR1} Km/Sec	U_{SCR1} Km/Sec	P_{SCR1} Kbars	T_R °C °K	U_{CR2} Km/Sec	U_{SCR2} Km/Sec	P_{SCR2} Kbars
TNT* (S.C.)	25 298 (RT)	1.654 (TMD)	2.30	2.25	with ΔH_T (melt)	0.6977	3.8698	44.65	300 573 T_{EXPL}	~	~	~
TNT* (S.C.)	25 298 (RT)	1.654 (TMD)	3.00	1.58	with ΔH_T (melt)	~	~	~	300 573 T_{EXPL}	0.9867	4.5589	74.40
TNT* (CAST) ↓	25 298 (RT)	1.614	2.39	2.05	with ΔH_T (melt)	0.6977	3.8203	43.02	300 573 T_{EXPL}	0.9867	4.4127	70.27
TNT** (PRESSED) ↓	18 291 (RT)	1.635	2.08	2.35	with ΔH_T (melt)	0.4066	3.0355	20.18	80.5 353.5 T_{MELT}	0.5750	3.4313	32.26

Table 7. $U_{P_{CR}}$ and $P_{S_{CR}}$ Comparison for TNT C_P and N/G C_P

			EXPERIMENTAL C_P				NOMINAL C_P					
ITEM	T_{EXP}	T_R	Up_{CR1}	Ps_{CR1}	Up_{CR2}	Ps_{CR2}	Up_{CR1}	Ps_{CR1}	Up_{CR2}	Ps_{CR2}	$\frac{\Delta U_{P_{CR}}}{U_P^{(EXP)}}$ *	$\frac{\Delta P_{S_{CR}}}{P_{S_{CR}}^{(EXP)}}$ **
~	°C/°K	°C/°K	Km/Sec	Kbars	Km/Sec	Kbars	Km/Sec	Kbars	Km/Sec	Kbars	PERCENT	PERCENT
TNT (S.C.) CASE 1	25/298 (RT)	300/573 (E_{XPL})	0.7502	49.48	1.0609	82.06	0.6977	44.65	0.9867	74.40	-7.0	-9.76 -9.33
TNT (CAST) CASE 1	25/298 (RT)	300/573 (E_{XPL})	0.7502	47.56	1.0609	78.16	0.6977	43.02	0.9867	70.27	-7.0	-9.54 -10.09
TNT (PRESSED) CASE 2	18/291 (RT)	80.5/353.5 (melt)	0.4152	20.74	0.5872	33.22	0.4066	20.18	0.5750	32.26	-2.07	-2.70 -2.89

$$* \frac{\Delta U_{P_{CR}}}{U_P^{(EXP)}} = \frac{U_{P_{CR}}(N/G) - U_{P_{CR}}(EXP)}{U_{P_{CR}}(EXP)} \quad X\ 100.0$$

$$** \frac{\Delta P_{S_{CR}}}{P_{S_{CR}}^{(EXP)}} = \frac{P_{S_{CR}}(N/G) - P_{S_{CR}}(EXP)}{P_{S_{CR}}(EXP)} \quad X\ 100.0$$

Table 8. Computation of $U_{P_{CR1}}$ and $U_{P_{CR2}}$ From Experimental C_P for PBX-9502

ITEM ~	m_{AV}	T_{EXP}	T_R	Remarks	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	ΔH_T	$\Delta(v.e.)_{TR}$	$\frac{\Delta(v.e)_{TR}}{m_{av}}$	Up_{CR1}	Up_{CR2}
~	Grams $*10^{-23}$	°C °K	°C °K	~	Cals $*10^{-23}$	Joules $*10^{-23}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$(Cm/Sec)^2$ $*10^{+10}$	Km/Sec	Km/Sec
PBX-9502	1.82118	-55 218	396 669 (T_{EXPL})	No ΔH	280.4168	1,173.264	1.173264	0.00	1.173264	0.64423	0.8026	1.1351
PBX-9502	1.82118	20 293 RT	396 669 (T_{EXPL})	No ΔH	247.8165	1,036.864	1.036864	0.00	1.036864	0.56933	0.7545	1.0671
PBX-9502	1.82118	75 348	396 669 (T_{EXPL})	No ΔH	220.0683	920.7658	0.9207658	0.00	0.9207658	0.50559	0.7110	1.0056
PBX-9502	1.82118	252 525	396 669 (T_{EXPL})	No ΔH	108.7080	454.8343	0.4548343	0.00	0.4548343	0.24975	0.4997	0.7067

Note: This Table is from Reference 5.

Table 9. Computation of Us_{CR} and Ps_{CR} From Experimental C_P for PBX-9502

ITEM ~	T_{EXP} °C ° K	ρ_O Grams/Cm^3	C_O Km/Sec	S ~	Remarks	Up_{CR1} Km/Sec	Us_{CR1} Km/Sec	Ps_{CR1} Kbars	T_R °C ° K	Up_{CR2} Km/Sec	Us_{CR2} Km/Sec	Ps_{CR2} Kbars
PBX-9502	-55 218	1.910	3.31	1.65	No ΔH	0.8026	4.6343	71.042	396 669 (T_{EXPL})	1.1351	5.1351	112.368
PBX-9502	20 293 (RT)	1.891	Non - Linear See Ref.5.		No ΔH	0.7545	4.1433	59.115	396 669 (T_{EXPL})	1.0671	4.8166	97.193
PBX-9502	75 348	1.857	2.60	1.91	No ΔH	0.7110	3.9580	52.259	396 669 (T_{EXPL})	1.0056	4.5207	84.419
PBX-9502	252 525	1.700	1.33	3.08	No ΔH	0.4997	2.8691	24.373	396 669 (T_{EXPL})	0.7067	3.5066	42.128

Note: This Table is from Reference 5.

Table 10. Computation of $U_{P_{CR1}}$ and $U_{P_{CR2}}$ From N/G C_P for PBX-9502

ITEM ~	m_{AV}	T_{EXP}	T_R	Remarks	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	ΔH_T	$\Delta(v.e.)_{TR}$	$\frac{\Delta(v.e)_{TR}}{m_{av}}$	Up_{CR1}	Up_{CR2}
~	Grams $*10^{-23}$	°C °K	°C °K	~	Cals $*10^{-23}$	Joules $*10^{-23}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$(Cm/Sec)^2$ $*10^{+10}$	Km/Sec	Km/Sec
PBX-9502	1.82118	-55 218	396 669 (T_{EXPL})	No ΔH	271.8287	1,137.331	1.137331	0.00	1.137331	0.6245	0.7903	1.1176
PBX-9502	1.82118	20 293 RT	396 669 (T_{EXPL})	No ΔH	242.5748	1,014.933	1.014933	0.00	1.014933	0.5573	0.7465	1.0472
PBX-9502	1.82118	75 348	396 669 (T_{EXPL})	No ΔH	216.7526	906.8929	0.9068929	0.00	0.9068929	0.4980	0.7057	0.9980
PBX-9502	1.82118	252 525	396 669 (T_{EXPL})	No ΔH	108.5578	454.2059	0.4542059	0.00	0.4542059	0.2494	0.4994	0.7063

Table 11. Computation of Us_{CR} and Ps_{CR} From N/G C_P for PBX-9502

ITEM ~	T_{EXP} °C °K	ρ_O Grams/Cm^3	C_O Km/Sec	S ~	Remarks	Up_{CR1} Km/Sec	Us_{CR1} Km/Sec	Ps_{CR1} Kbars	T_R °C °K	Up_{CR2} Km/Sec	Us_{CR2} Km/Sec	Ps_{CR2} Kbars
PBX-9502	-55 218	1.910	3.31	1.65	No ΔH	0.7903	4.6140	69.65	396 669 (T_{EXPL})	1.1176	5.1540	110.02
PBX-9502	20 293 (RT)	1.891	Non - Linear See Ref.5.		No ΔH	0.7465	4.1235	58.21	396 669 (T_{EXPL})	1.0557	4.7948	95.72
PBX-9502	75 348	1.857	2.60	1.91	No ΔH	0.7057	3.9479	51.74	396 669 (T_{EXPL})	0.9980	4.5062	83.51
PBX-9502	252 525	1.700	1.33	3.08	No ΔH	0.4994	2.8682	24.35	396 669 (T_{EXPL})	0.7063	3.5054	42.09

Table 12. $U_{P_{CR}}$ and $P_{S_{CR}}$ Comparison for PBX-9502 C_P and N/G C_P

			PBX-9502 C_P				NOMINAL C_P					
ITEM	T_{EXP}	T_R	Up_{CR1}	Ps_{CR1}	Up_{CR2}	Ps_{CR2}	Up_{CR1}	Ps_{CR1}	Up_{CR2}	Ps_{CR2}	$\frac{\Delta U_{PCR}}{U_P{}^{(EXP)}}$ *	$\frac{\Delta P_{SCR}}{P_{SCR}{}^{(EXP)}}$ **
~	°C/°K	°C/°K	Km/Sec	Kbars	Km/Sec	Kbars	Km/Sec	Kbars	Km/Sec	Kbars	PERCENT	PERCENT
PBX-9502	$-55/218$	$396/669$	0.8026	71.042	1.1351	112.368	0.7903	69.65	1.1176	110.02	-1.54	-1.96 (1) -2.09 (2)
PBX-9502	$20/293$	$396/669$	0.7545	59.115	1.0671	97.193	0.7465	58.21	1.0557	95.72	-1.06	-1.53 (1) -1.52 (2)
PBX-9502	$75/348$	$396/669$	0.7110	52.259	1.0056	84.419	0.7057	51.74	0.9980	83.51	-0.75	-0.99 (1) -1.08 (2)
PBX-9502	$252/525$	$396/669$	0.4997	24.373	0.7067	42.128	0.4994	24.35	0.7063	42.09	-0.06	-0.09 (1) -0.09 (2)

Note: No ΔH included.

$$* \frac{\Delta U_{PCR}}{U_{PCR}{}^{(EXP)}} = \frac{U_{PCR}(N/G) - U_{PCR}(EXP)}{U_{PCR}(EXP)} \times 100.0$$

$$** \frac{\Delta P_{SCR}}{P_{SCR}{}^{(EXP)}} = \frac{P_{SCR}(N/G) - P_{SCR}(EXP)}{P_{SCR}(EXP)} \times 100.0$$

Table 13. Computation of $U_{P_{CR1}}$ and $U_{P_{CR2}}$ From Experimental C_P for HMX

ITEM ~	m_{AV}	T_{EXP}	T_R	Remarks	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	ΔH_T	$\Delta(v.e.)_{TR}$	$\frac{\Delta(v.e)_{TR}}{m_{av}}$	Up_{CR1}	Up_{CR2}
~	Grams $*10^{-23}$	°C °K	°C °K	~	Cals $*10^{-23}$	Joules $*10^{-23}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$(Cm/Sec)^2$ $*10^{+10}$	Km/Sec	Km/Sec
HMX	1.75633	27 300 RT	287 560 T_{DEFL}	with ΔH_T $\beta \rightarrow \delta$	148.7849	622.5160	0.62252	0.05515 $\beta \rightarrow \delta$	0.67767	0.3858	0.6212	0.8785

Note: This information is from Reference 3.

Table 14. Computation of Us_{CR} and Ps_{CR} From Experimental C_P for HMX

ITEM ~	T_{EXP} °C °K	ρ_O Grams/Cm^3	C_O Km/Sec	S ~	Remarks	Up_{CR1} Km/Sec	Us_{CR1} Km/Sec	Ps_{CR1} Kbars	T_R °C ° K	Up_{CR2} Km/Sec	Us_{CR2} Km/Sec	Ps_{CR2} Kbars
HMX	27 300 RT	1.891	3.07	1.79	with ΔH_T $\beta \rightarrow \delta$	0.6212	4.1820	49.13	287 560 T_{DEFL}	0.8785	4.6425	77.12

Note: This information is from Reference 3.

Table 15. Computation of $U_{P_{CR1}}$ and $U_{P_{CR2}}$ From N/G C_P for HMX

ITEM ~	m_{AV}	T_{EXP}	T_R	Remarks	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	$\int_{T_{EXP}}^{T_R} C_p dT$	ΔH_T	$\Delta(v.e.)_{TR}$	$\frac{\Delta(v.e)_{TR}}{m_{av}}$	Up_{CR1}	Up_{CR2}
~	Grams $*10^{-23}$	°C °K	°C °K	~	Cals $*10^{-23}$	Joules $*10^{-23}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$G(Cm/Sec)^2$ $*10^{-13}$	$(Cm/Sec)^2$ $*10^{+10}$	Km/Sec	Km/Sec
HMX	1.75633	27 300 RT	287 560 T_{DEFL}	with ΔH_T $\beta \rightarrow \delta$	156.7975	656.0407	0.6560407	0.05515 $\beta \rightarrow \delta$ [3]	0.7111907	0.40493	0.6363	0.8999

Table 16. Computation of Us_{CR} and Ps_{CR} From N/G C_P for HMX

ITEM ~	T_{EXP} °C °K	ρ_O Grams/Cm^3	C_O Km/Sec	S ~	Remarks	Up_{CR1} Km/Sec	Us_{CR1} Km/Sec	Ps_{CR1} Kbars	T_R °C ° K	Up_{CR2} Km/Sec	Us_{CR2} Km/Sec	Ps_{CR2} Kbars
HMX	27 300 RT	1.891	3.07	1.79	with ΔH_T $\beta \rightarrow \delta$	0.6363	4.2090	50.64	287 560 T_{DEFL}	0.8999	4.6808	79.65

Table 17. $U_{P_{CR}}$ and $P_{S_{CR}}$ Comparison for HMX C_P and N/G C_P

			Experimental C_P				NOMINAL C_P					
ITEM	T_{EXP}	T_R	U_{PCR1}	P_{SCR1}	U_{PCR2}	P_{SCR2}	U_{PCR1}	P_{SCR1}	U_{PCR2}	P_{SCR2}	$\frac{\Delta U_{PCR}}{U_P{}^{(EXP)}}$ *	$\frac{\Delta P_{SCR}}{P_{SCR}{}^{(EXP)}}$ **
~	°C/°K	°C/°K	Km/Sec	Kbars	Km/Sec	Kbars	Km/Sec	Kbars	Km/Sec	Kbars	PERCENT	PERCENT
HMX	27/300	287/560	0.6212	49.13	0.8785	77.12	0.6363	50.64	0.8999	79.65	+2.43	+3.07 (1) +3.28 (2)

Note: With ΔH_T ($\beta \rightarrow \delta$).

$$* \frac{\Delta U_{PCR}}{U_{PCR}{}^{(EXP)}} = \frac{U_{PCR}(N/G) - U_{PCR}(EXP)}{U_{PCR}(EXP)} \text{ X } 100.0$$

$$** \frac{\Delta P_{SCR}}{P_{SCR}{}^{(EXP)}} = \frac{P_{SCR}(N/G) - P_{SCR}(EXP)}{P_{SCR}(EXP)} \text{ X } 100.0$$

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